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Combined mollification—future temperatures procedure for solution of inverse heat conduction problem

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Abstract: The inverse heat conduction problem involves the calculation of surface heat flux and/or temperature histories from transient, measured temperatures inside solids. This paper proposes and investigates a new combined procedure that is based on two different methods: a data filtering interpretation of the mollification method and Beck's future temperature method. A test case is investigated of a semi-infinite body exposed to a heat flux that is initially zero, has a unit increase, an then drops to zero. The combined procedure is shown to be accurate and stable with respect to perturbations in the data even for small dimensionless time steps. The future temperatures method can be significantly improved upon by the combined procedure.

Keywords: Ill-posed problems, heat transfer conduction

1. Introduction

In several practical contexts, it is sometimes necessary to estimate the surface heat flux and/or temperature histories from transient, measured temperatures inside solids. The inverse heat conduction problem (IHCP) is frequently encountered, for example, in the determination of thermal constants in some quenching processes, the estimation of surface heat transfer measurements taken within the skin of a re-entry vehicle, the determination of aerodynamic heating in wind tunnels and rocket nozzels, the design and development of calorimeter-type instrumentation, the experimental determination of thermophysical properties of materials, and infrared computerized axial tomography.

The IHCP is a mathematically improperly posed problem because the solution does not depend continuously upon the data, that is, small errors in the interior data induce large errors in the surface heat flux or in the surface temperature solutions.

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Several researchers have examined the IHCP and a number of different solution methods have been reported in the literature (see, e.g., the comprehensive account given in [2] and the references there in). By attempting to reconstruct a slightly "mollified" or "filtered" image of the unknowns, Manselli and Miller [5] and Murio [6] have shown that it is possible to restore certain type of continuous dependence on the data. In what follows, this method is called the mollification method (MM). Beck [1,2] has attempted to stabilized the ICHP using several future-time temperatures with a least-squares method to calculate components of the heat flux of temperature at a given time. Hereafter, this method is called the "future-temperature" method (FT).

The methods mentioned above are sequential methods. They lead very naturally to a step-by-step algorithm and, consequently, they are computationally efficient.

In this paper, a new sequential method is introduced by combining a different interpretation of the MM method, originally suggested by Hensel and Hills [4] and further developed by Murio [7], and Beck's "future-temperatures" method. The aim is to incorporate the better stability properties of the MM method, see [6], to the simple algorithm describing the FT method. The combined method (MM–FT) should be stable and accurate even for small dimensionless time steps ($\Delta t \approx 0.01$), a very desirable property that the FT method above fails to satisfy, see [3]. At the same time, it is expected that the MM–FT method will require, for small Δt's, a substantially smaller number of future temperatures than the FT method. This becomes an important practical detail, for example, in the actual implementation of the method for the numerical solution of the two dimensional IHCP.

Our approximation is generated initially by automatically filtering the noisy data by discrete convolution with a suitable averaging kernel and then using the FT method to numerically solve the associated well-posed (formally) problem. The purpose here is to investigate this method and to compare it with Beck's method for small time steps.

In Section 2, the semi-infinite one dimensional problem is presented and a stabilized version of the inverse problem is introduced. Section 3 describes the procedure that uniquely determines the radius of mollification depending on the amount of noise in the data. Section 4 presents a detailed description of the new algorithm. The efficiency of the combined method is demonstrated in Section 5 where we show the results of several computations analyzing the solution error as a function of the number of future temperatures for noisy data and small times steps. A comparison with the FT method is also included. Section 6 gives a summary and some conclusions.

2. Description of the problem

A semi-infinite slab is considered to illustrate the method.

After obtaining a measured transient temperature history $\bar{f}(t)$ at the interior point $x = 1$, it is desired to recover the boundary heat flux $q(t)$.

Linear heat conduction with constant thermal properties is considered. Without loss of generality, the problem is normalized by using dimensionless quantities.

The unknown temperature $u(x, t)$ satisfies

$$u_t = u_{xx}, \qquad 0 < x < \infty, \quad 0 < t < \infty, \tag{1a}$$

$$u(1, t) = f(t) \tag{1b}$$

with corresponding approximate data function $\bar{f}(t)$, $0 < t < \infty$,

$$u(x, 0) = 0, \quad 0 \leqslant x < \infty, \tag{1c}$$

$$-u_x(0, t) = q(t), \qquad 0 \leqslant t < \infty, \quad \text{unknown}, \tag{1d}$$

$$u(x, t) \quad \text{bounded as } x \to \infty, \tag{1e}$$

where t is time and x is the distance measured from the heated surface.

Equation (1) is equivalent to the Volterra integral equation of the first kind

$$f(t) = \int_0^t q(s) \frac{\partial \phi(1, t-s)}{\partial t} \, \mathrm{d}s, \tag{2}$$

where $\phi(1, t)$, the temperature response at $x = 1$ for a unit step rise of the surface heat flux at $t = 0$, is given by

$$\phi(1, t) = \begin{cases} \dfrac{2}{\sqrt{\pi}} \sqrt{t} \exp(-1/4t) - \operatorname{erfc}(1/2\sqrt{t}), & t > 0, \\ 0, \quad t \leqslant 0. \end{cases} \tag{3}$$

It is well known that the solution of (2) depends discontinuously upon the data. Since in any practical situation f is not known exactly and only a measured (noisy) approximation $\bar{f}$ is available, small errors in the experimental data may cause large errors in the solution q.

In order to use some results from Fourier integral analysis, we extend $f(t)$, $\bar{f}(t)$ and $q(t)$ to the whole real t-axis by defining f, $\bar{f}$ and q to be zero for $t < 0$. We assume that all the functions involved are L^2-functions in $(-\infty, \infty)$, and use the corresponding L^2-norm to measure errors. In this setting, it is quite natural to also assume that the unknown function $q(t)$ satisfies the L^2-data error bound

$$\| (k * q)(t) - \bar{f}(t) \| = \| f(t) - \bar{f}(t) \| \leqslant \epsilon, \tag{4}$$

where we have introduced the notation

$$k(1, t-s) = \partial \phi(1, t-s)/\partial t. \tag{5}$$

Under these hypotheses, it is shown in [6] that the inverse problem can be stabilized if, instead of attempting to find the point values of q, we attempt to reconstruct the δ-mollification of q at time t, given by

$$J_\delta q(t) \equiv (p_\delta * q)(t), \tag{6}$$

where

$$p_\delta(t) = \frac{1}{\delta\sqrt{\pi}} \, \mathrm{e}^{-t^2/\delta^2} \tag{7}$$

is the Gaussian kernel of radius $\delta > 0$. We notice that p_δ and $J_\delta q$ are C^∞ (infinitely differentiable) functions in $(-\infty, \infty)$, with $p_\delta \geqslant 0$ and $\int_{-\infty}^{+\infty} p_\delta(s) \, \mathrm{d}s = 1$. The function p_δ falls to nearly zero outside a few δ radii from its center ($\approx 3\delta$). Moreover, the Fourier transform of $J_\delta q$,

$$\hat{J}_\delta q(w) = 2\pi \hat{p}_\delta(w) \cdot \hat{q}(w) = \mathrm{e}^{-w^2\delta^2/4} \hat{q}(w), \tag{8}$$

shows that the mollification in (6) damps those Fourier components of q with wavelength $2\pi/\omega$ much shorter than $2\pi\delta$; the longer wavelengths are damped hardly at all.

With $J_\delta q$ and $J_\delta \bar{q}$ denoting the δ-mollifications of the heat fluxes associated with the exact data $f(t)$ and the measured data $\bar{f}(t)$ respectively, the following Lemma is proved in [6].

Lemma 1. *If* $\|(k * q)(t) - \bar{f}(t)\| \leqslant \epsilon$, *then*

$$|J_\delta q(t) - J_\delta \bar{q}(t)| \leqslant \frac{\sqrt{2}}{\sqrt{\pi}} \frac{\epsilon}{\delta} \exp(1/\sqrt{2\delta}).$$

This shows that attempting to reconstruct the linear functional $J_\delta q(t)$ at some time t of interest and for some assigned radius $\delta > 0$, is a formally stable problem with respect to perturbations in the data. The error is guaranteed to go to zero as $\epsilon \to 0$ for fixed δ.

From (2), (6), and (5) it follows that the δ-mollification of the surfact heat flux, $J_\delta q$, satisfies

$$\begin{aligned}(p_\delta * f)(t) &= (p_\delta * (k * q))(t) \\ &= (k * (p_\delta * q))(t) = (k * J_\delta q)(t),\end{aligned} \tag{9}$$

a formally stable version of equation (2) with $f(t)$ replaced by a suitable filtered data function $J_\delta f(t) = (p_\delta * f)(t)$. This is a new interpretation of the MM method, suggested in [4]. The succesful implementation of the filtering procedure, i.e., the automatic determination of the radius of mollification, δ, as a function of the amount of noise in the data, ϵ, was investigated in [6] and it is discussed in the next section.

3. Automatic selection of the radius of mollification

In this section we indicate a procedure to determine the radius of mollification, δ, based on properties of the filtered data function $p_\delta * \bar{f}$.

The mollification of the data function $\bar{f}$ by convolution with the kernel p_δ is actually an averaging process that satisfies

Lemma 2. *If* $\delta_1 > \delta_2 > 0$, *then* $\| J_{\delta_1}\bar{f} - \bar{f}\| > \| J_{\delta_2}\bar{f} - \bar{f}\|$.

Proof. It follows immediately from equations (6) and (7), using Fourier transforms, the convolution theorem, Parseval's identity and the fact that $\| J_\delta \bar{f} - \bar{f}\| \to 0$ as $\delta \to 0$. □

The monotonicity property in Lemma 2 shows that there is a unique $\bar{\delta}$ such that

$$\| J_{\bar{\delta}}\bar{f} - \bar{f}\| = \epsilon. \tag{10}$$

The parameter selection criterion introduced by (10) determines $\hat{\delta}$ in a manner which is consistent with the amount of work in the data function $\bar{f}$. Furthermore, the bisection method can easily be implemented to numerically determine $\hat{\delta}$. We notice that in actual computations, only a finite data record of $\bar{f}$ is available. Without loss of generality, let us assume that the data function $\bar{f}$ is known only in the interval $I = [0, 1]$. We need to extend the data function to the whole real line in such a way that $\bar{f}(t)$ decays smoothly to zero for $1 < t < 1 + a$ for some $a > 0$ and it is zero for $t \geqslant 1 + a$. For instance, we can define

$$f(t) = f(1) \exp\left[(t-1)^2/\left((t-1)^2 - a\right)\right], \quad 1 \leqslant t \leqslant 1 + a. \tag{11}$$

With the data function extended as indicated, the radius of mollification $\hat{\delta}$ is now determined by solving

$$\| J_\delta \bar{f} - \bar{f} \|_I = \epsilon. \tag{12}$$

The computational details are presented in the next section.

4. Numerical procedure

Since in practice only a discrete set of points is generally available, we assume in what follows that the data function $\bar{f}$ is a discrete function in $I = [0,1]$, measured at the $N+1$ sample points $t_i = i\ \Delta t$, $i = 0, 1, \ldots, N$; $N\Delta t = 1$. Given $a > \Delta t$, we use (11) to extend the data to $[0,1+a]$ and because the data is defined to be zero for $t \leqslant 0$ and $t \geqslant 1 + a$, we consider the extended discrete data function $\bar{f}$ defined at equally spaced sample points on any interval of interest containing I.

The parameter selection is implemented by solving the discrete version of (12) using the bisection method. The following steps summarized the algorithm.

Step 1. Let $\delta_{\min} = \Delta t$, $\delta_{\max} = 0.5$ and choose an initial value of δ between $\delta_{\min}$ and $\delta_{\max}$.

Step 2. Compute $J_\delta \bar{f} = \rho_\delta * \bar{f}$ by discrete convolution on a sufficiently large interval containing the interval I.

Step 3. If

$$F(\delta) = \left[\frac{1}{N+1} \sum_{i=1}^{N} \left(J_\delta \bar{f}(t_i) - \bar{f}(t_i) \right)^2 \right]^{1/2} = \epsilon \pm \eta,$$

where η is a given tolerance, exit.

Step 4. If $F(\delta) - \epsilon < -\eta$, set $\delta_{\min} = \delta$. If $F(\delta) - \epsilon > \eta$, set $\delta_{\max} = \delta$. The updated value of δ is always given by $(\delta_{\min} + \delta_{\max})/2$.

Step 5. Return to Step 2.

Once the radius of mollification $\hat{\delta}$ and the discrete filtered data function $J_{\hat{\delta}} \bar{f}$ are determined, we need to numerically solve the integral equation

$$J_{\hat{\delta}} \bar{f}(t) = \int_0^t J_{\hat{\delta}} q(s) \frac{\partial \phi(l, t-s)}{\partial t}\, \mathrm{d}s \tag{13}$$

to approximately compute the discrete function $J_{\hat{\delta}} q$ at the grid points of interest. Here we use the FT method [1,2].

The integral equations (13) can be approximated at time t_M by

$$J_\delta f_M = \sum_{n=0}^{M-1} J_\delta \hat{q}_n \Delta\phi_{M-n} - J_\delta q_M \Delta\phi_0, \quad J_\delta q_0 = 0, \tag{14}$$

where

$$J_\delta f_M = J_\delta f(M\,\Delta t), \qquad \Delta\phi_i = \phi((i+l)\Delta t) - \phi(i\Delta t), \qquad J_\delta q_n = J_\delta q((n-1/2)\Delta t).$$

The caret on q_n denotes a previously estimated value of a mollified heat flux component. The only unknown in (14) is $J_\delta q_M$, which is to be estimated in a sequential manner.

The temperature at times $(M+j)\ \Delta t$, $j = 0, 1, 2, \ldots$ is given by

$$J_\delta f_{M+j} = \sum_{n=0}^{M-1} J_\delta \hat{q}_M\ \Delta\phi_{M-n+j} + J_\delta q_M\ \Delta\phi_j + \cdots + J_\delta q_{M+j}\ \Delta\phi_0. \tag{15}$$

The mollified heat flux at time $(M+i-\frac{1}{2})\ \Delta t,\ i=1, 2,\ldots$ may be expressed at

$$J_\delta q_{M+i}=A_0+A_l i+A_2 i^2+\cdots+A_\beta i^\beta \tag{16}$$

and the coefficient A_0, which is equal to $J_\delta q_M$, is to be found. If $\beta=0$, the heat flux is constant, and, if $\beta=1$, there is a linear variation of the surface heat flux.

Assuming that the maximum value of j in (15) is equal to $r-1$, then it is required that

$$S_r=\sum_{j=0}^{r-1}\left(J_\delta f_{M+j}-J_\delta\bar{f}_{M+j}\right)^2 \tag{17}$$

be made a minimum with respect to $A_0,\ A_1,\ldots,\ A_\beta$. To obtain a solution, r must be at least as large as $\beta+1$ and, in order to introduce some least-squares smoothing, it is necessary that $r\geqslant\beta+2$. Equation (17) uses r future temperatures to obtain the single mollified heat flux component $J_\delta q_M$.

Differentiation of (15) with respect to Ap gives the set of linear equations

$$\sum_{j=0}^{r-1}\left(J_\delta f_{M+j}-J_\delta\bar{f}_{M+j}\right)C_{pj},\quad p=0, 1,\ldots,\beta, \tag{18}$$

where

$$C_{pj}=\sum_{l=0}^{j} l^p\ \Delta\phi_{j-l},\quad p=0, 1,\ldots,\beta.$$

This set of equations is equivalent to

$$\sum_{i=0}^{\beta}\alpha_{ip}A_i=\gamma_p,\quad p=0, 1,\ldots,\beta \tag{19}$$

where

$$\alpha_{ip}=\alpha_{pi}=\sum_{j=0}^{r-1}c_{ij}c_{pj},\qquad i=0, 1,\ldots,\beta,\quad p=0, 1,\ldots,\beta,$$

$$\gamma_p=\sum_{j=0}^{r-1}J_\delta\bar{f}_{M+j}C_{pj}-\sum_{n=0}^{M-1}\left(J_\delta q_n\sum_{j=0}^{r-1}\Delta\phi_{M-n+j}C_{pj}\right),\quad J_\delta q_0\equiv 0.$$

After Δt, β and r are chosen ($r\geqslant\beta+2$), the set of $\beta+1$ linear equations given by (19) is solved for A_0. This solution is then taken as the accepted value of $q(t)$ over the Mth single time step only. Next, the right hand side of (19) is updated, the analysis interval is shifted one time step, and the entire process is repeated. For $\beta=0$ (piecewise constant solution), there is just one linear equation with one unknown and, if $\beta=1$ (piecewise linear solution), a system of two linear equations with two unknowns is obtained. It should be mentioned that the future temperatures method outlined above has been traditionally applied directly to the noisy data $\bar{f}$ instead of the mollified or filtered data $J_\delta\bar{f}$.

The algorithm described in this section successfully combines the mollification method (MM) and Beck's future temperatures method (FT).

5. Numerical results

In this section we discuss the implementation of the combined (MM–FT) method.

In order to test the accuracy of the method, the approximate reconstruction of a surface heat flux $q(t)$ is investigated for a semi-infinite body exposed to a heat flux of value 1 between $t = 0.2$ and $t = 0.6$ and of value 0 at other times. Such a curve has the difficult characteristics of an abrupt rise and an equally abrupt drop and constitutes a severe test because the algorithm anticipates changes in the heat flux and gives delayed values.

The time interval of interest is always $I = [0,1]$ and the discrete data function is extended to $[0,1 + a]$, as explained in Section 4, with $a = 0.1$. The exact temperature data is denoted by $f(t)$ and the noisy data, $\bar{f}(t)$, is obtained by adding a random error to $f(t_i)$, $t_i = i\,\Delta t$, $i = 0, 1, \dots, N$; $N\,\Delta t = 1$. Thus,

$$\bar{f}(t_i) = f(t_i) + \epsilon_i, \tag{21}$$

where ϵ_i is a Gaussian random variable of variance ϵ^2. The exact data temperature for this problem is

$$f(t) = \phi(1,\ t - 0.2) - \phi(1,\ t - 0.6).$$

The average perturbations used in our tests are for $\epsilon = 0.01$ and corresponds to approximately

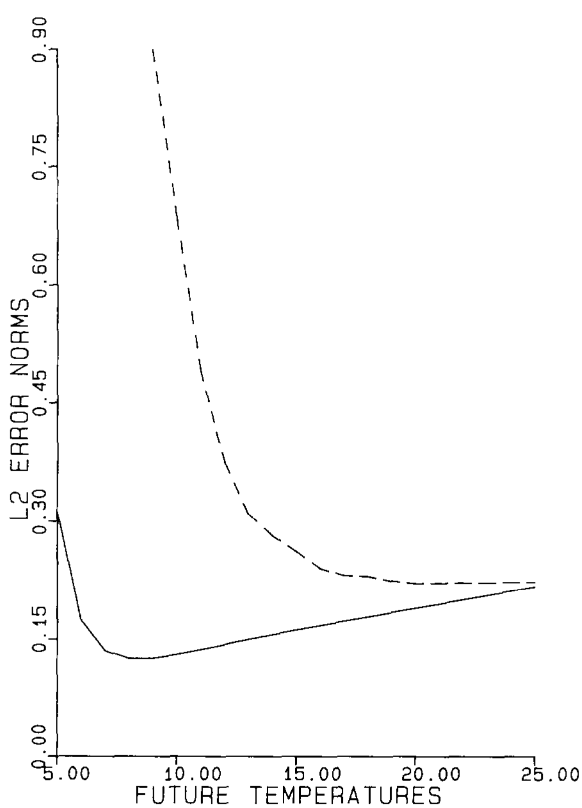

Fig. 1. L_2 Error Norms. $\epsilon = 0.01$, $\Delta t = 0.01$, $\beta = 0$. FT method (— — —)($\delta = 0$). MM-FT method (———)($\hat{\delta} = 0.02$).

5% of the maximum data temperature which is about 0.2. After extending the discrete data function, the parameter selection criterion was implemented with the tolerance η, used in Step 3 of the procedure, set to reflect a 5% error in the satisfaction of the constraint. Independently of the initial choice of δ, convergence to the value $\hat{\delta} = 0.02$ was reached in no more than 8 iterations.

If the discretized computed heat flux component is denoted by $J_\delta q_i$ and the true component is q_i, in order to measure the error, we introduce the sample root mean square norm of the error, given by

$$E_\delta = \left[\frac{1}{N+1} \sum_{i=0}^{N} (J_\delta q_i - q_i)^2 \right]^{1/2}, \quad N\,\Delta t = 1. \tag{22}$$

For a small dimensionless time step ($\Delta t = 0.01$) and constant heat flux assumption ($\beta = 0$), it is shown in Fig. 1 (dashed line) that, without data filtering ($\delta = 0$), the optimal number of future temperature which minimize (22) using the FT method is $r = 20$. The associated error is approximately 0.21. Using the same parameters and the combined MM–FT method with $\hat{\delta} = 0.02$, the error is reduced to approximately 0.18. For the MM–FT method, the optimal number of future temperatures which minimizes the sample root mean square norm of the error

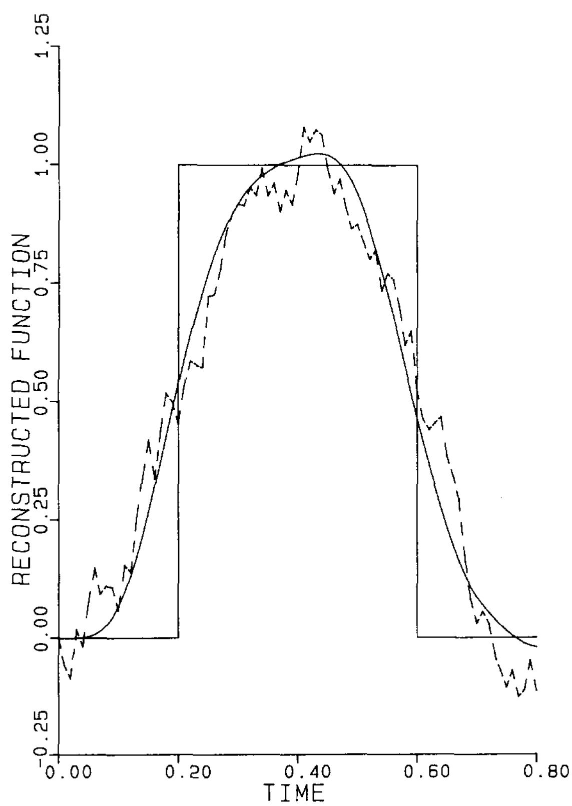

Fig. 2. Reconstructed surface heat flux. $\epsilon = 0.01$, $\Delta t = 0.01$, $\beta = 0$, $r = 20$. FT method (— — —)($\delta = 0$). MM–FT method (———)($\hat{\delta} = 0.02$).

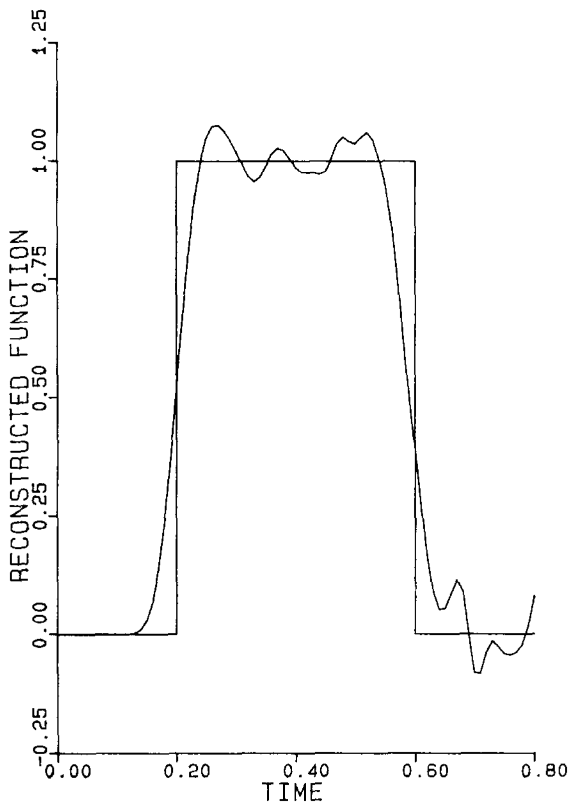

Fig. 3. Reconstructed surfact heat flux. $\epsilon = 0.01$, $\Delta t = 0.01$, $\beta = 0$, $r = 8$. MM–FT method (———)($\hat{\delta} = 0.02$).

is $r = 8$, as shown in Fig. 1 (full line). The qualitative behavior of the reconstructed surface heat fluxes is plotted in Fig. 2 for $r = 20$ with dashed line for the FT method and full line for the combined MM–FT method. Figure 3 shows the reconstructed surface heat flux using the combined MM–FT method and $r = 8$ future temperatures. In this case, $E_{0.02} \approx 0.12$. We observe, as expected, the total absence of numerical instability. Furthermore, the resolution in this case is quite good considering the relative high noise level that we used.

6. Conclusions

A new interpretation of the mollification method that leads very naturally to a discrete convolution filtering technique that automatically adjusts the radius of mollification to the amount of noise in the data is successfully combined with Beck's sequential function specification or future-temperatures method. The combined method is still sequential and thus computationally efficient.

A test case is investigated for a constant surface heat flux assumption and for small dimensionless time step ($\Delta t = 0.01$). The sample root mean square norm of the error is studied as a function of the number of future temperatures.

The combined sequential method is compared with Beck's method and for random error corresponding to $\epsilon = 0.01$, the combined method performs better than the future temperatures method. The optimal number of future temperatures decreases from about 20 to 8 and the error also decreases significantly from about 0.21 to 0.12.

A general conclusion is that the sequential function specification method can be improved upon by the combined procedure. The latter is considerably more stable and accurate.

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